LA-UR -79-1902

TITLE: AN APPLICATION OF PADE APPROXIMANTS TO ELASTIC WAVE SCATTERING

AUTHOR(S): James Edward Gubernatis

SUBMITTED TO: ARPA/AF Review of Progress in Quantitative NDE, July 8-13 Scripps Institution of Oceanography

MASTER

los alamos scientific laboratory of the University of California
LOS ALAMOS, NEW MEXICO 87545

UNITED STATES
ENERGY RESEARCH AND
DEVELOPMENT ADMINISTRATION
CONTRACT W-7405-ENG. 36

AN APPLICATION OF PADÉ APPROXIMANTS TO ELASTIC WAVE SCATTERING

J. E. GUBERNATIS
THEORETICAL DIVISION
LOS ALAMOS SCIENTIFIC LABORATORY
LOS ALAMOS, NEW MEXICO 87545

ABSTRACT

Several Padé methods were used to try to accelerate the convergence of partial wave sums for scattering amplitudes. A specific test problem of longitudinal-to-longitudinal scattering from a spherical void was studied in detail. Results for this test case and the behavior of partial wave amplitudes for general cases are presented and discussed.

INTRODUCTION

Recently, numerical procedures,[1-4] based on the method of eigenfunctions expansions, were devised to calculate the scattering of an elastic wave from a flaw. If the shape of the flaw is axially symmetric, then these procedures are efficient, accurate and easily implemented. Their implementation requires only a computer of modest memory; their coding, standard numerical techniques; and the execution of the code, small amounts of computer time. However, if the flaw is generally shaped, practical concerns impede their implementation. The principal impediment is the need to compute and store more information. In general, the computing time and storage requirements are at least an order of magnitude greater. Simply using a bigger, faster computer is generally inadequate; a computer system with "virtual" memory (or very fast discs) and more sophisticated coding techniques are needed. Furthermore, the calculation becomes expensive.

The present investigation sought a method to permit the use of the eigenfunction expansion techniques for generally-shaped flaws without the need of bigger, faster computers and more sophisticated coding techniques and still permit an inexpensive calculation. Simply stated, a method was sought that would take whatever information the eigenfunction expansion techniques could practically yield and then extrapolate this information into an accurate scattering result.

In detail, one wants to calculate a scattering amplitude. The exact scattering amplitude A is a complex number which in terms of a partial-wave eigenfunction expansion is

$$A(\theta,\phi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} a_{\ell m} Y_{\ell m}(\theta,\phi) \tag{1}$$

where the $a_{\ell m}$ are partial wave scattering amplitudes, $Y_{\ell m}$ are spherical harmonics, and θ and ϕ are scattering angles. The eigenfunction expansion techniques give the $a_{\ell m}$, and the object of these techniques is to compute enough $a_{\ell m}$ so the sequence of partial sums for $A(\theta,\phi)$, i.e.

$$A_L = \sum_{\ell=0}^{L} \sum_{m=-\ell}^{\ell} a_{\ell m} Y_{\ell m}(\theta,\phi) \tag{2}$$

converges to some required accuracy, e.g.

$$|A_L - A_{L-1}| < \epsilon |A_{L-1}| \tag{3}$$

where ϵ is a relative error criterion. The object of present investigation is to take unconverged information and mathematically extrapolate it to approximate $A(\theta,\phi)$ to required accuracy. To do this, various approximations theories, classified as Padé Approximants, were studied and used on a specific test problem. This problem was the calculation of longitudinal-to-longitudinal scattering of a plane wave from a spherical cavity. For this problem the exact scattering amplitude[5] has a simple partial wave expansion,

$$A(\theta) = \sum_{\ell=0}^{\infty} a_\ell P_\ell(\cos\theta) \tag{4}$$

where the $P_\ell(\cos\theta)$ are Legendre polynomials and the partial wave amplitudes a_ℓ are known in terms of simple, analytic expressions. The partial sums

$$A_L = \sum_{\ell=0}^{L} a_\ell P_\ell(\cos\theta) \tag{5}$$

were easily computed to a relative error of $\epsilon = 10^{-12}$.

The initial Padé Approximants studied were ones recently developed in nuclear physics.[6-12] They are very successful for accelerating the convergence partial sums (4) for the scattering from large classes of long and short-ranged potentials. These techniques are generalizable to two variable partial wave sums, i.e. (2).

PADÉ APPROXIMANTS

The Padé Approximant.[13] The [M/N] Padé Approximant to a function F(x) is

$$F^{[M/N]}(x) = P_M(x)/Q_N(x) \tag{6}$$

where $P_M(x)$ is a polynomial of degree at most M and $Q_N(x)$ is a polynomial of degree at most N. If F(x) has the formal power series expansion

$$F(x) = \sum_{\ell=0}^{\infty} f_\ell x^\ell \tag{7}$$

and $P_M(x)$ and $Q_N(x)$ are

$$P_M(x) = p_0 + p_1 x + \ldots + p_M x^M \tag{8a}$$

$$Q_N(x) = 1 + q_1 x + \ldots + q_N x^N \tag{8b}$$

Then the equation

$$Q_N(x) F(x) - P_M(x) = O(x^{M+N+1}) \tag{9}$$

completely and uniquely determines the M+1 coefficients of $P_M(x)$ and N coefficient of $Q_N(x)$ in terms of the first M+N+1 coefficients of the power series expansion of F(x). Specifically, one carries out the implied power series multiplications in (9), equates terms of like powers of x, and then solves an M+N+1 set of linear algebraic equations for the p's and q's in terms of the f's.

Padés have numerous uses, but their use in summing series is of immediate interest. In this use, one takes the first M+N+1 coefficients in a partial sum of

$$F_{M+N} = \sum_{\ell=0}^{M+N} f_\ell x^\ell \tag{10}$$

computes various sequences of Padés, and examines their convergence. For certain classes of functions the Padés must converge to the correct answer. For many other classes of functions for which convergence proofs are absent experience shows that if the Padés converge, they converge to the correct answer.

It is helpful to be mindful that in the construction of (6) only the coefficients of a partial sum of the infinite series in (7) is used. However, (6) has the formal power series expansion

$$F^{[M/N]}(x) = \sum_{\ell=0}^{\infty} f_\ell^{[M/N]} x^\ell \tag{11}$$

and it is easy to show the first M+N+1 coefficients of this series equal the first M+N+1 coefficients of (7). The higher order coefficients in (11) approximate the higher order coefficients in (7). With respect to (7) these higher order coefficients were not used to construct (6). This is useful if the higher order terms are unknown, slowly convergent, or too expensive to calculate. The idea is to get the Padé to approximate them for us.

<u>Generalized Padé Approximants.</u>[13] The generalized Padé Approximant (or Baker-Gammel Approximants) apply to functions G(x) which have the representation

$$G(x) = \sum_{\ell=0}^{\infty} g_\ell k_\ell(x) \tag{12}$$

where

$$k_\ell(x) = \frac{1}{\ell!}\left[\left(\frac{\partial}{\partial x}\right)^\ell K(x,u)\right]_{u=0} \tag{13}$$

with the generating function K(x,u) to be specified. For example, if $K(x,u) = (1 - 2xu + u^2)^{\frac{1}{2}}$

$$G(x) = \sum_{\ell=0}^{\infty} g_\ell P_\ell(x) \tag{14}$$

where $P_\ell(x)$ is the Legendre polynomial. The [M+J/M] generalized Padé Approximant to G(x) is

$$G^{[M+J/M]}(x) = \sum_{j=0}^{J} \beta_j k_j(x) + \sum_{j=1}^{M} \alpha_j K(x,u_j) \tag{15}$$

with the j-summation absent if J = -1. The β_j, α_j and u_j are to be specified. When the generating function for Legendre polynomials is used for K(x,u), the generalized approximants are called <u>Legendre-Padé Approximants.</u>[6]

One way to specify the β_j, α_j, and u_j is with the g_ℓ in (12) to create the formal series

$$F(x) = \sum_{\ell=0}^{\infty} g_\ell x^\ell$$

and then construct $F^{[M+J/M]}(x)$. It then can be shown that

$$g_\ell = \beta_\ell + \sum_{j=1}^{M} \alpha_j u_j^\ell, \quad \ell = 0, 1, \ldots, J \tag{16a}$$

and

$$g_\ell = \sum_{j=1}^{M} \alpha_j u_j^\ell, \quad \ell = J+1, J+2, \ldots, 2M+J \tag{16b}$$

That is, the β_j, α_j and u_j are unknowns in a nonlinear system of equations with the known constants g_ℓ. More conveniently, it can also be shown that u_j^{-1} and α_j/u_j are the poles and residues of $F^{[M/N]}(x)$, and β_j, the coefficients in the series expansion of $F^{[M+J/M]}(x)$ as $x \to \infty$. All these quantities (the poles, residues, etc.) are easily obtained by simple numerical analysis. The generalized approximant (15) has the property that

$$G^{[M+J/M]}(x) = \sum_{\ell=0}^{\infty} g_\ell^{[M+J/M]} k_\ell(x) \tag{17}$$

with the first 2M+J+1 terms identical to the first such terms in (12). Again, the Padé Approximant has taken the coefficients in a partial sum and returned them plus an approximation for the remaining coefficients of the actual infinite sum.

<u>n-Point Padé Approximants.</u>[13] If a function F(x) has the values $F_1, F_2, \ldots, F_n$ at $x_1, x_2, \ldots, x_n$ then the n-Point [M/N] Padé Approximant (or the Lagrange interpolation polynomials) is the ratio of two polynomials of degree at most M and N

$$F^{[M/N]}(x) = P_M(x)/Q_N(x) \tag{18}$$

so that

$$F^{[M/N]}(x_i) = F_i, \quad i = 1, 2, \ldots, n \tag{19}$$

(P_M and Q_N are defined as in (8).)

Of immediate interest is the 1-Point (or Punctual[10]) Padé Approximant. This approximation applies to the sum

$$B = \sum_{\ell=0}^{\infty} b_\ell \tag{20}$$

and its partial sums.

$$B_L = \sum_{\ell=0}^{L} b_\ell \tag{21}$$

Now if one considers the formal power series

$$F(x) = \sum_{\ell=0}^{\infty} b_\ell \, x^\ell \tag{22}$$

then $B = F(1)$. The 1-Point [M/N] Padé Approximant to (20), i.e. $B^{[M/N]}$, is constructed by forming $F^{[M/N]}(x)$ for (21) (i.e. find the p's and q's) and equating

$$B^{[M/N]} = F^{[M/N]}(1) = \sum_{m=0}^{M} p_m \Big/ \left(1 + \sum_{n=1}^{N} q_n\right) \tag{23}$$

The approximants $B^{[M/N]}$ are equivalent to Shanks's[14] formal generalization of Aitken's extrapolation formula. This approximation is applied to partial wave sums by defining

$$b_\ell = a_\ell \; P_\ell(\cos \theta) \tag{24}$$

RESULTS

To achieve the same degree of accuracy, the various Padé methods used were found to need at least as many partial wave coefficients as the partial sums. The Padé methods investigated afford no computational advantage over directly summing the series.

In Fig. 1 the magnitudes of the partial sum (5) are plotted as a function of L. As a reminder, the test problem is the longitudinal-to-longitudinal scattering of a plane wave from a spherical cavity; $A(\theta)$ is the scattered amplitude; a is the radius of the sphere; and k is the incident and scattered wavenumber. (For the partial sum A_L, L+1 coefficients are needed.) Figure 1 shows that for different values of ka the partial sums behave similarly. Each sequence rises monotonically to a plateau. For each ka, there is a particular L which marks the beginning of the plateau (L=2, 5, and 10). For these L's the partial sum has a

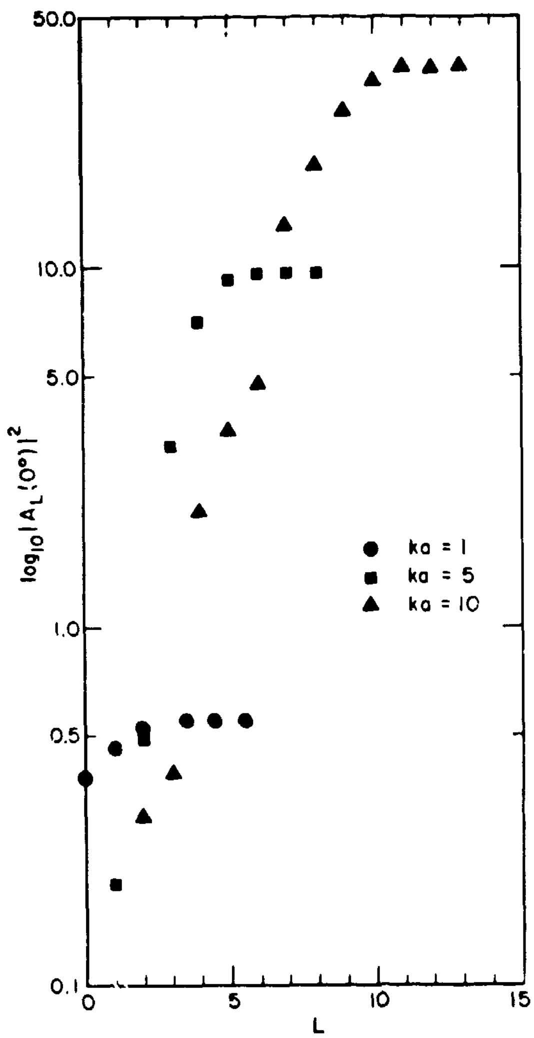

Fig. 1. The convergence of the forward scattering differential cross-section as a function of L.

relative error $\epsilon = 10^{-2}$. For smaller L values the partial sums are bad approximations to the exact answer; for larger L values the partial sum converges rapidly. The sums achieve a $\epsilon = 10^{-12}$ for L=8, 17 and 25 when ka = 1, 5 and 10.

The Padé methods behave similarly: Convergence starts abruptly and then proceeds rapidly. This behavior is listed in Tables I, II and III for ka = 1, 5 and 10. (The [M/N] need M+N+1 coefficients.) Except for [M-1/M] all sequences [N/M] for $N \geq M$ and a given method behave as those listed;

Table I. The longitudinal differential cross-section at $\theta = 0°$ and ka = 1 for three diagonal sequences of the 1-Point, Legendre and Asymptotic Legendre Padé Approximants.

	1-POINT			LEGENDRE			ASYMPTOTIC LEGENDRE		
M	[M-1/M]	[M/M]	[M+1/M]	[M-1/M]	[M/M]	[M+1/M]	[M-1/M]	[M/M]	[M+1/M]
1	0.3814	0.5021	0.5705	0.3814	0.5021	0.5705	0.4448	0.5198	0.5570
2	0.5492	0.5517	0.5333	0.5492	0.5517	0.5533	0.5560	0.5533	0.5530
3	0.5536	0.5533	0.5533	0.5536	0.5533	0.5533	0.5533	0.5533	0.5533
4	0.5533	0.5533	0.5533	0.5533	0.5533	0.5533	0.5533	0.5533	0.5533

Table II. The longitudinal differential cross-section at $\theta = 0°$ and ka = 5 for three diagonal sequences of the 1-Point, Legendre and Asymptotic Legendre Padé Approximants.

	1-POINT			LEGENDRE			ASYMPTOTIC LEGENDRE		
M	[M-1/M]	[M/M]	[M+1/M]	[M-1/M]	[M/M]	[M+1/M]	[M-1/M]	[M/M]	[M+1/M]
1	0.0077	0.1447	0.4000	0.0077	0.1447	0.3648	0.1850	0.4060	7.4391
2	0.0283	0.6722	8.7317	0.0104	0.1084	8.7317	5.8718	9.0470	12.5913
3	0.6091	2.4488	9.6990	0.1889	1.7738	9.6990	9.8046	9.3165	9.5915
4	14.1791	9.6471	9.6179	14.1791	9.6471	9.6179	9.5810	9.6143	9.6179
5	9.5925	9.6209	9.6179	9.5925	9.6209	9.6179	9.6178	9.6179	9.6179
6	9.6195	9.6179	9.6179	9.6195	9.6179	9.6179	9.6179	9.6179	9.6179
7	9.6179	9.6179	9.6179	9.6179	9.6179	9.6179	9.6179	9.6179	9.6179

furthermore, the behavior is essentially independent of scattering angle. We note that for ka = 10 the 1-Point and Legendre Padé methods need more coefficients than the partial sum to achieve $\epsilon = 10^{-12}$.

In all cases the partial sums converge when L > ka. To try to understand the behavior of these sums, the behavior of the coefficients a_ℓ were studied. In particular, their behavior for $\ell >> ka$ was found.[5] For a spherical void and inclusion

$$a_\ell \underset{\ell \to \infty}{\to} \frac{i^\ell (ka)^{2\ell-2}}{[(2\ell+1)!!]^2} \equiv c_\ell (ka)^{2\ell-2} \tag{25}$$

If one lets

$$d_\ell = a_\ell / c_\ell \tag{26}$$

then

$$\frac{1}{(ka)^2} \left| \frac{d_\ell}{d_{\ell-1}} \right|_{\ell \to \infty} \to 1 \tag{27}$$

The left-hand side of the above is plotted in Fig. 2 as a function of ℓ. From this figure one sees that for ℓ = 8 and 17 (for ka = 1 and 5), the ratio has approached its asymptotic limit. (Actually the limits are still several percent away.) For ka = 10 the limit is not yet attained. For these ℓ values the ϵ for the partial sums is 10^{-12}.

Figures 1 and 2 and (25) suggest the following: Although the partial wave coefficients eventually fall off very rapidly, this rapid fall-off (or asymptotic behavior) occurs after the rapid convergence of the partial sum. The behavior of the partial wave coefficients needed in a converged partial sum is quite different than the asymptotic behavior. The Padé methods might be ineffective because of this. What was devised is a new Padé method, the Asymptotic Legendre-Padé Approximant,[15] which utilizes the asymptotic behavior of the partial wave coefficients. The Padé coefficients are forced to anticipate the correct asymptotic behavior so hopefully the convergence of predicted partial wave summation is accelerated.

The Asymptotic Legendre-Padé can be constructed in the following way: For the Legendre series

$$A(\theta) = \sum_{\ell=0}^{\infty} a_\ell P_\ell(\cos\theta)$$

instead of constructing the [M+J/M] Legendre Padé from the convergent series

$$F(x) = \sum_{\ell=0}^{\infty} a_\ell x^\ell$$

construct it from the divergent series

$$F(x) = \sum_{\ell=0}^{\infty} d_\ell x^\ell$$

that is with the asymptotic behavior divided out. (d_ℓ is given by (25) and (26).) After constructing the [M+J/M] Padé, one has

$$F^{[M+J/M]}(x) = \sum_{\ell=0}^{\infty} d_\ell^{[M+J/M]} x^\ell \tag{28}$$

Then,

Table III. The longitudinal differential cross-section at $\theta = 0°$ and ka = 10 for three diagonal sequences of the 1-Point, Legendre and Asymptotic Legendre Padé Approximants.

	1-POINT			LEGENDRE			ASYMPTOTIC LEGENDRE		
M	[M-1/M]	[M/M]	[M+1/M]	[M-1/M]	[M/M]	[M+1/M]	[M-1/M]	[M/M]	[M+1/M]
1	0.0003	0.0291	0.2877	0.0003	0.0291	0.2877	0.0382	0.2756	0.3434
2	0.0224	0.0942	0.4015	0.0081	0.0210	0.0541	0.3732	0.3488	0.3637
3	0.0733	0.6031	1.5343	0.0335	0.1820	0.4131	3.6676	10.5304	25.9765
4	1.4516	1.3077	2.4237	0.3678	0.4141	0.6907	25.9288	31.8504	53.5930
5	3.5562	4.3865	2.6270	3.9362	1.0873	0.7402	53.1786	41.1073	48.3262
6	0.0879	2.2731	1.7432	0.0385	0.7730	0.4011	49.3442	36.5396	36.0059
7	0.9116	2.3716	76.5076	0.4305	1.2012	76.5076	36.0028	35.8575	35.8543
8	0.1463	24.1183	35.8899	0.0597	24.1183	35.8899	35.8543	35.8518	35.8518
9	48.5999	35.8766	35.8515	48.5999	35.8766	35.8515	35.8518	35.8519	35.8518
10	35.8242	35.8517	35.8518	35.8242	35.8517	35.8518	35.8518	35.8519	35.8518
11	35.8518	35.8518	35.8518	35.8518	35.8518	35.8543	35.8518	35.8518	35.8518
12	35.8518	35.8516	35.8518	35.8518	35.8518	35.8514	35.8518	35.8518	35.8518

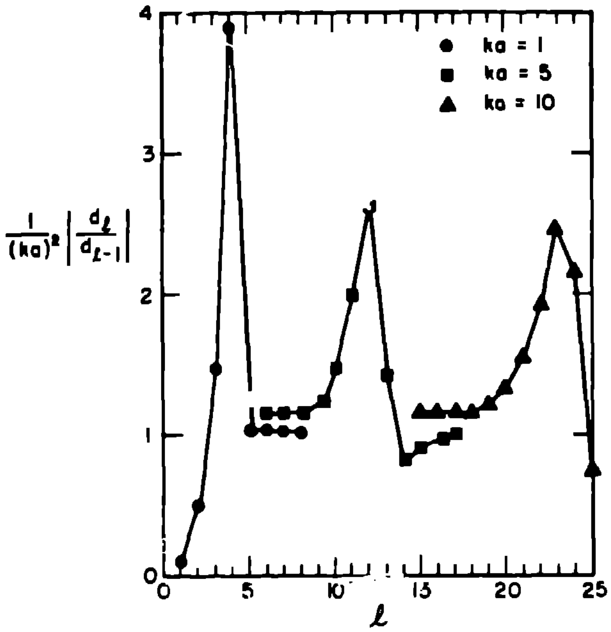

Fig. 2. The convergence of the partial wave amplitudes to their asymptotic value as a function of L. (See (27) in text.)

$$A^{[M+J/M]} = \sum_{\ell=0}^{\infty} a_\ell^{[M+J/M]} P_\ell(\cos\theta) \tag{29}$$

where

$$a_\ell^{[M+J/M]} = d_\ell^{[M+J/M]} c_\ell \tag{30}$$

(The analysis can be made more formal by specifying a $K(x,u)$.)

The results of the application of the new method are also listed in Tables I, II and III. For ka = 10 (Table III) this new method converges faster than the 1-Point and Legendre-Padés; however, the convergence is still no faster than the partial sum.

DISCUSSION

Clearly, not all possible summation techniques were studied and those studied were applied to a specific flaw shape. However, the 1-Point and Legendre-Padé Approximants are "state-of-the-art" for nuclear physics scattering problems. The Asymptotic Legendre-Padé Approximant, developed for this investigation, will probably advance the state-of-the-art.

Why do the techniques work for nuclear scattering and not for elastic wave scattering? There is an important difference between the scattering problems studied in nuclear physics and the problem studied here. For the problem under discussion the flaw (or scatterer) is modeled as a finite, homogeneous region of space. The corresponding scatterer in nuclear physics is the square-well potential. This is a short-ranged potential; however, the short-ranged potentials to which the Padé methods are being successfully applied are families of the Yukawa potential. For the pure Yukawa potential, the asymptotic behavior of its partial wave amplitudes is[16]

$$a_\ell \propto \frac{(2\ell+1)!}{[(2\ell+1)!!]^2}(ka)^{2\ell+1} \tag{31}$$

which does not fall off as rapidly as (25). For the square-well potential[16]

$$a_\ell \propto \frac{(ka)^{2\ell+1}}{[(2\ell+1)!!]^2(2\ell+3)} \tag{32}$$

which is quite similar to (25). The partial sums for square-well-type potential apparently converges too fast for the Padé methods to be advantageous over the partial sums.

The asymptotic behavior in (25) is apparently not limited to spherical flaws. For generally-shaped flaws, the Born approximation provides a useful estimate of the asymptotic behavior of the partial wave coefficients.[16] One has

$$A(\theta,\phi) \propto \int_{\text{flaw}} dV\, e^{i(\underline{k}-\underline{k}_0)\cdot\underline{r}} \tag{33}$$

where $\underline{k}$ and $\underline{k}_0$ are the scattered and incident wave vectors. Since

$$e^{i\underline{k}\cdot\underline{r}} = 4\pi \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} i^\ell j_\ell(kr) Y^*_{\ell m}(\theta_k,\phi_k) Y_{\ell m}(\theta_r,\phi_r) \tag{34}$$

then

$$A(\theta,\phi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} a_{\ell m} Y_{\ell m}(\theta,\phi) \tag{35}$$

where

$$a_{\ell m} \propto \int_{\text{flaw}} dV\, j_\ell^2(kr) \simeq V j_\ell^2(kR) \tag{36}$$

with V being the volume of the flaw and R some characteristic length of the flaw. For $\ell \gg kR$

$$j_\ell(kR) \to \frac{(kR)^\ell}{[(2\ell+1)!!]} \tag{37}$$

Hence as $\ell \to \infty$

$$a_{\ell m} \propto \frac{(kR)^{2\ell}}{[(2\ell+1)!!]^2} \tag{38}$$

which is very similar to (25). Again the above estimate and (25) is independent of the flaw being a void or inclusion. One can easily convince oneself that the finite volume of the flaw, not its homogeneity, is the significant factor for the rapid fall-off.

Equation (38) implies that the partial wave expansion, even for generally shaped objects, is quite rapidly convergent. However, question is not whether the sum converges, but how many terms are needed? The goal was to produce an accurate sum with no more than ten terms.

Just because the Padé techniques afford no computational advantage when the flaw is spherical does not prove that the techniques will be as ineffective for non-spherical flaws. What is needed is a clearer picture how the partial wave sums behave for non-spherical flaws. There are few studies of the convergence properties of the eigenfunction expansion method. There is some indication that for a spheroidal flaw the partial sums behave at least differently; furthermore, different implementations of the eigenfunction expansion method may converge differently.[2]

ACKNOWLEDGEMENTS

It is my pleasure to acknowledge helpful discussions with George A. Baker, Jr.

REFERENCES

1. W. M. Visscher, Los Alamos Scientific Laboratory Report 78-3008 (1978); J. Appl. Phys. (in press).

2. W.M. Visscher, Los Alamos Scientific Laboratory Report 79-0399 (1979); J. Appl. Phys. (in press).

3. P.C. Waterman, J. Acost. Soc. Am. 60 567 (1976).

4. V. Varatharajulu and Y.-H. Pao, J. Acost. Soc. Am. 60 556 (1976).

5. C.F. Ying and R. Truell, J. Appl. Phys. 27, 1086 (1956).

6. A.K. Common and T. Stacey, J. Phys. A 11, 259 (1978).

7. A.K. Common and T. Stacey, "The Convergence of Legendre-Padé Approximants to Coulomb and Other Scattering Amplitudes," unpublished.

8. A.K. Common, "Calculation of Yukawa Scattering and Impact Parameter Amplitudes using Legendre-Padé Approximants," unpublished.

9. C.R. Garibotti and F.F. Grinstein, J. Math Phys. 19, 2405 (1978).

10. C.R. Garibotti and F.F. Grinstein, J. Math Phys. 19, 821 (1978).

11. C.R. Garibotti and F.F. Grinstein, "Summation of Partial Wave Expansions in the Scattering by Long Range Potentials: II. Numerical Applications," unpublished.

12. F.F. Grinstein, "Summation of Partial Wave Expansions in the Scattering by Short Range Potentials, "unpublished.

13. George A. Baker, Jr. Essentials of Padé Approximants, (Academic Press, New York, 1975).

14. D. Shanks, J. Phys. and Math. (Mass.) 34, 1 (1955).

15. G.A. Baker, Jr. and J.E. Gubernatis, unpublished.

16. K. Gottfried, Quantum Mechanics, Vol. 1, (W.A. Benjamin, Inc., New York, 1966), Chap. III.